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DEPENDENCE OF THE ELECTRON ENERGY DISTRIBUTION ON THE VIBRATIONAL TEMPERATURE IN THE ELECTRICALLY EXCITED N₂

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ABSTRACT

The effects of the vibrational excitation and deexcitation of nitrogen molecules in an electrical discharge on the electron energy distributions and transport coefficients are investigated theoretically. The electrons collide with vibrationally excited molecules either gain or lose energy which results in the redistribution of the electron energy. The distribution function is calculated numerically by solving the Boltzmann equation, using a complete set of elastic momentum transfer and inelastic cross sections. The presence of vibrationally excited molecules which collide and exchange energy with the electrons has a strong effect on the electron energy distribution function. This effect is demonstrated for various vibrational temperatures. The energy distributions are calculated at the ratio of electric field to gas density E/N which ranges from 10^{-16} to $20 \times 10^{-16} \text{ V cm}^2$. Generally, as the vibrational temperature increases, the electrons become richer in the high-energy tail of the distribution function.

I. INTRODUCTION

The evolution of the electrical conductivity generated by a propagating relativistic charged particle beam in a neutral gaseous medium has been an interesting subject for many years. The ionization of the gas by charged particle beams generates secondary electrons which either lose or gain the energy through elastic and inelastic collisions with the gas species. The conductivity of the plasma channel can be determined if one knows the electron energy distribution, which results from the interaction of the plasma with molecules and beam induced electromagnetic fields. For simplicity, it is often convenient to assume that the electron velocity distribution is Maxwellian. However, the degree of accuracy of the Maxwellian assumption depends on the plasma conditions and the magnitude of E/N .

Numerical calculations of the electron energy distribution in typical electrical discharge in N_2 have been studied by many authors¹⁻⁵ by solving the Boltzmann equation. Nitrogen was chosen because of its high abundance in the atmosphere. Besides, the cross sections for the elementary processes in nitrogen have been studied and well documented.⁶ Once the energy distribution function is obtained, the transport coefficients, such as the electron drift velocity, the ratio of the diffusion coefficient to the electron mobility D/u (the characteristic energy) etc. are obtained in the usual manner. In general the results show that the calculated transport coefficients are in good agreement with the experiment.⁷⁻⁹ Most of all, the calculated distribution functions are found to be markedly non-Maxwellian.¹⁻⁵

In most practical cases, however, the fractional population of the vibrationally excited molecules in an electric discharge can be very significant, while the density of electronically excited molecules is still low.⁹ Electron collisions with the vibrationally excited molecules can

result in the excitation (or deexcitation) to higher (or lower) vibrational levels. As the vibrational temperature increases, the molecules have a substantial degree of vibrational excitation. It is the purpose of this paper to take into account the presence of highly populated vibrationally excited molecules which modify the electron energy distribution because of the electron inelastic and superelastic collisions with the molecules. The aim of this paper is to demonstrate that one must account for superelastic collisions with the vibrationally excited molecules to obtain the proper electron energy distribution. In certain cases one must also consider the superelastic collisions with the electronic states. However, this will be the subject of a future paper.

II. THEORY

In the electron energy distribution calculations, the conventional two-term spherical harmonic expansion¹ is chosen to represent the angular dependence of the electron distribution in the velocity space. Accordingly the Boltzmann equation for a spatially independent electron swarm in a spatially uniform gas under the influence of a steady electric field E can be expressed as¹

$$\frac{d}{du} \left[\frac{E^2 u}{3N^2 Q_m(u)} \frac{df_0(u)}{du} \right] + \frac{2m}{M} \frac{d}{du} [u^2 Q_m(u) (f_0 + \frac{KT}{e} \frac{df_0}{du})] \quad (1)$$

$$= - \sum_{\ell, k} [(u + u_{\ell k}) f_0(u + u_{\ell k}) X_{\ell} Q_{\ell k}(u + u_{\ell k}) - u f_0(u) X_{\ell} Q_{\ell k}(u)]$$

$$- \sum_{\ell, k} [(u - u_{\ell k}) f_0(u - u_{\ell k}) X_{\ell} Q_{k\ell}(u - u_{\ell k}) - u f_0(u) X_{\ell} Q_{k\ell}(u)]$$

where $f_0(u)$ is the isotropic component of the electron energy distribution function with electron energy u expressed in electron volts, N the gas density, K the Boltzman constant, e the electron charge and T the gas temperature. M and m are the mass of the gas molecule and the electron, respectively. Q_m is the electron - N_2 momentum transfer cross section. $Q_{\ell k}$ refers to vibrational and electronic excitation and ionization cross sections, $u_{\ell k}$ is the characteristic energy loss for each process, and X_{ℓ} is the fractional concentration of the ℓ th species. The second term on the right hand side will be retained only if the corresponding deexcitation is present and $Q_{k\ell}$ is the cross section. Equation (1) can be reduced by integrating once with respect to u which yields the result

$$\frac{E^2 u}{3N^2 Q_m(u)} \frac{df_0(u)}{du} + \frac{2m}{M} u^2 Q_m(u) \left[f_0(u) + \frac{KT}{e} \frac{df_0(u)}{du} \right] \quad (2)$$

$$= - \sum_{l,k} \int_u^{u+u_{lk}} u f_0^X Q_{lk} du + \sum_{lk} \int_{u-u_{lk}}^u u f_0^X Q_{kl} du$$

where u_{lk} is defined as the energy loss for a collision in which the molecule changes its vibrational state from l to k . Equation (2) is a first-order integrodifferential equation which can be solved numerically. The numerical method described in Appendix V of Reference 1 is used for the present calculation.

III. NUMERICAL RESULTS

Let us consider the case where the fractional concentration of vibrationally excited molecules is so low that the effect of their presence on the electron energy distribution can be neglected. Consequently, the second term on the right hand side of Eq. (2) is omitted because no deexcitation is being considered. In other words, the nitrogen molecules are all in the ground state so that $X_l = 1$. In practice, the subscripts l can be eliminated entirely in Eq. (2). This Boltzmann transport equation can be integrated numerically using the backward prolongation technique of Sherman.¹⁰

The processes considered include rotational, vibrational and electronic excitation, ionization and dissociation. For vibrational excitations only the first eight levels are considered. The energy loss by the ionization and dissociate ionization is treated as one of the excitation processes. A complete set of electron cross section data was used in solving the Boltzmann equation numerically for the steady state condition. The electron energy distributions for various values of E/N are shown in Fig. 1. The E/N values are varied from $1 - 20 \times 10^{-16} \text{ V cm}^2$, corresponding to mean electron energies approximately from 1 to 5 eV. The calculated distributions show the important features of the electron energy loss in N_2 . Because of the peak value of the vibrational cross sections near 2 eV, it is difficult for the electrons to obtain larger energies to pass over the vibrational barrier. Note that the distribution function $f_0(u)$ has been normalized as in Eq. (3)

$$\int_0^{\infty} u^{1/2} f_0(u) du = 1. \quad (3)$$

For each distribution function the calculated drift velocity W , the characteristic energy D/μ and the average electron energy E_{av} are listed below:

E/N (V cm ²)	W (cm/sec)	D/μ	E_{av} (eV)
1.0×10^{-16}	1.79×10^6	0.98	0.96
2.0×10^{-16}	3.00×10^6	1.17	1.04
5.0×10^{-16}	6.27×10^6	1.38	1.15
1.0×10^{-15}	1.07×10^7	2.02	2.23
1.5×10^{-15}	1.48×10^7	2.96	3.80
2.0×10^{-15}	1.87×10^7	3.74	5.02

If the Maxwellian function is normalized as indicated by Eq. (3), then the energy distribution becomes

$$f(u) = 2\pi^{-1/2} T_e^{-3/2} e^{-u/T_e}, \quad (4)$$

where T_e is the average electron temperature expressed in electron volts. Therefore the Maxwellian distribution functions for any T_e would appear in the log-linear plot as a straight line. For comparison we plot in Fig. 2 the Maxwellian functions corresponding to each curve in Fig. 1. It is obvious that the calculated electron energy distribution functions are non-Maxwellian. However, it seems that $f_0(u)$ tend to be more Maxwellian as E/N increases. Clearly the resulting energy distributions have shown the important features of the electron-molecule energy exchange processes in the electrically excited N_2 . In Fig. 3 we show the calculated electron excitation

rate coefficients for eight ground state vibrational levels of N_2 . At low E/N , most of the energy is dissipated into the vibrational excitations. Also shown in Fig. 3 are the equivalent excitation rates obtained by assuming a Maxwellian energy distribution.¹¹ It can be seen obviously that the Maxwellian distribution is not a good approximation for calculating these rate coefficients until E/N exceeds $3 \times 10^{-15} \text{ V cm}^2$.

We now consider the influence of the vibrationally excited molecules on the electron energy distribution. If the molecules have a substantial degree of vibrational excitation, one must take into account the superelastic collisions of the electrons with the vibrationally excited molecules. In other words, the excitation and deexcitation should be considered at the same time. For simplicity, we assume that the vibrational states are in a Boltzmann distribution where their fractional concentration for each vibrational state λ can be expressed as

$$X_\lambda \equiv N_\lambda / N_{\text{total}} = (1 - e^{-0.3/T_v}) e^{-0.3\lambda/T_v}, \quad (5)$$

where T_v is the vibrational temperature. Equation (2) has to be solved in full with the right hand side representing collisions of the first and second kind. If $T_v = 0$ then $X_\lambda = 0$ for every λ except $\lambda = 0$. That is exactly the case of no vibrational excitation just discussed. The entire matrix of cross sections for vibrational excitation and deexcitation are related by Eqs. (6) and (7)

$$Q_{i,j} = Q_{0,j-i} \quad (6)$$

$$Q_{0,i}(u + u_{th})(u + u_{th}) = Q_{i,0}(u)u \quad \text{for } u > 0 \quad (7)$$

where $Q_{i,j}$ is defined as the cross section for a collision in which the molecule changes its vibrational state from i to j . In Eq. (7), use has been made of detailed balancing between collisions of the first and second kind. U_{th} is the threshold energy for vibrational excitation of the nitrogen molecule by electron impact from the ground state to i th vibrational state. For calculations of the distribution function with vibrationally excited molecules, the contribution to the right hand side of Eq. (2) due to the presence of the vibrational states from $\lambda = 0$ to 8 can be expressed as

$$S_{\lambda k} = \sum_{\lambda=0}^8 \left[- \sum_{k=\lambda+1}^8 \int_u^{u+u_{\lambda k}} u f_0 X_{\lambda} Q_{\lambda k} du + \sum_{k=0}^{\lambda-1} \int_{u-u_{\lambda k}}^u u f_0 X_{\lambda} Q_{k\lambda} du \right] \quad (8)$$

where the two terms represent the excitation and deexcitation of vibrationally excited molecules, respectively. Making use of Eqs. (6) and (7), Eq. (8) yields

$$S_{\lambda k} = \sum_{\lambda=0}^8 X_{\lambda} \left[- \sum_{k=\lambda+1}^8 \int_u^{u+u_{\lambda k}} u f_0 Q_{\lambda k} du + \sum_{k=0}^{\lambda-1} \int_u^{u+u_{\lambda k}} u f_0(u-u_{\lambda k}) Q_{k\lambda} du \right] \quad (9)$$

where the second term involves the distribution function $f_0(u - u_{\lambda k})$ which is unknown and causes some difficulty to use the backward prolongation technique to solve Eq. (2). Another method involving a matrix inversion is necessary to take care of this problem. However, since the second term can be omitted at $T_v = 0$, we can at least predict the solution of $f_0(u)$ at $T_v = 0$ using the

background prolongation technique. As T_v increases gradually, a predictor-corrector iterated procedure is used until $f_0(u)$ converges to steady state solution.

The electron energy distribution functions are calculated for various vibrational temperatures at the ratio of E/N range from 10^{-16} to $20 \times 10^{-16} \text{ V cm}^2$. The distribution functions for $E/N = 3 \times 10^{-16} \text{ V cm}^2$ are shown in Fig. 4 for various vibration temperatures. The effect of the vibrational temperature on the distribution starts to become important as $T_v > 0.04 \text{ eV}$. As the vibrational temperature increases, the vibrationally excited molecules transfer their excitational energy to electrons in collisions of the second kind, so that the electron energy distribution becomes relatively rich in the high energy portion of the distribution function. As a second example, we choose $E/N = 5 \times 10^{-16} \text{ V cm}^2$ and do the similar calculations. The results are shown in Fig. 5. The threshold of vibrational temperature for effecting the distribution curve is around 0.05 eV . As E/N increases, it seems that higher vibrational temperature is necessary to increase the high-energy electrons. Finally, in the case of $E/N = 10 \times 10^{-16} \text{ V cm}^2$ the distribution curves are shown in Fig. 6 with the vibrational temperature threshold near 0.1 eV . As T_v increases, there is a decrease in $f_0(u)$ in the $0 - 2 \text{ eV}$ range. The electrons gain a lot of energy from the vibrational deexcitation especially for such high vibrational temperature. The slow electrons gain sufficient energy to pass the barrier and become faster electrons. This results in an increase in the high-energy portion of the distribution function. However, as T_v continues to increase to 0.8 eV , the distribution curve near 2 eV tends to be more Maxwellian as clearly indicated in Fig. 6. Further increase in T_v beyond 0.8 eV makes minimal change in the energy distribution.

Finally, as to the dependence of the transport coefficients on the vibrational temperature, we found that the calculated electron drift velocities remain almost unchanged as the vibrational temperature increases. However, the characteristic energy and the average electron energy are strong functions of the vibrational temperature, especially for higher value of E/N . As an example, for $E/N = 10^{-15} \text{ V cm}^2$ Fig. 7 shows the calculated characteristic energy D/μ and the average electron energy E_{av} as a function of the vibrational temperature. The results indicate that vibrational temperature variations have an important influence on the high-energy portion of the electron distribution in electrically excited gases and thus on electronic excitation and ionization. Therefore the effect of the vibrational excitation and deexcitation of molecules on the electron energy distributions and transport coefficients can not be ignored.

The electron energy distribution functions and transport coefficients in molecular nitrogen are calculated for the moderate value of E/N range from 1×10^{-16} to 2×10^{-15} V cm². The calculations are carried out by numerically solving the Boltzmann equation, using a set of accurate electron-collision cross sections. The results indicate that the electron distribution is not Maxwellian and the corresponding electron impact excitation rate coefficients for eight ground state vibrational levels are significantly different from Maxwellian rates, especially for low E/N .

The emphasis of this study has been placed on the calculation of the distribution function in the presence of vibrationally excited molecules and the dependence of the electron energy distribution on the variation of vibrational temperature. The excitation as well as deexcitation processes have to be considered in order to obtain the true electron distribution function as our calculations clearly indicate.

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FIGURE CAPTIONS

- Fig. 1 The electron energy distributions for various values of E/N .
- Fig. 2 The Maxwellian functions corresponding to each curve in Fig. 1.
- Fig. 3 The calculated electron excitation rate coefficients for eight ground state vibrational levels of N_2 are compared to that obtained using a Maxwellian electron energy distribution.
- Fig. 4 The electron energy distribution functions for various temperatures when $E/N = 3 \times 10^{-16} \text{ V cm}^2$.
- Fig. 5 The electron energy distribution functions for various vibrational temperatures when $E/N = 5 \times 10^{-16} \text{ V cm}^2$.
- Fig. 6 The electron energy distribution functions for various vibrational temperatures when $E/N = 10^{-15} \text{ V cm}^2$.
- Fig. 7 The calculated characteristic energy D/μ and the average electron energy E_{av} as a function of vibrational temperature when $E/N = 10^{-15} \text{ V cm}^2$.

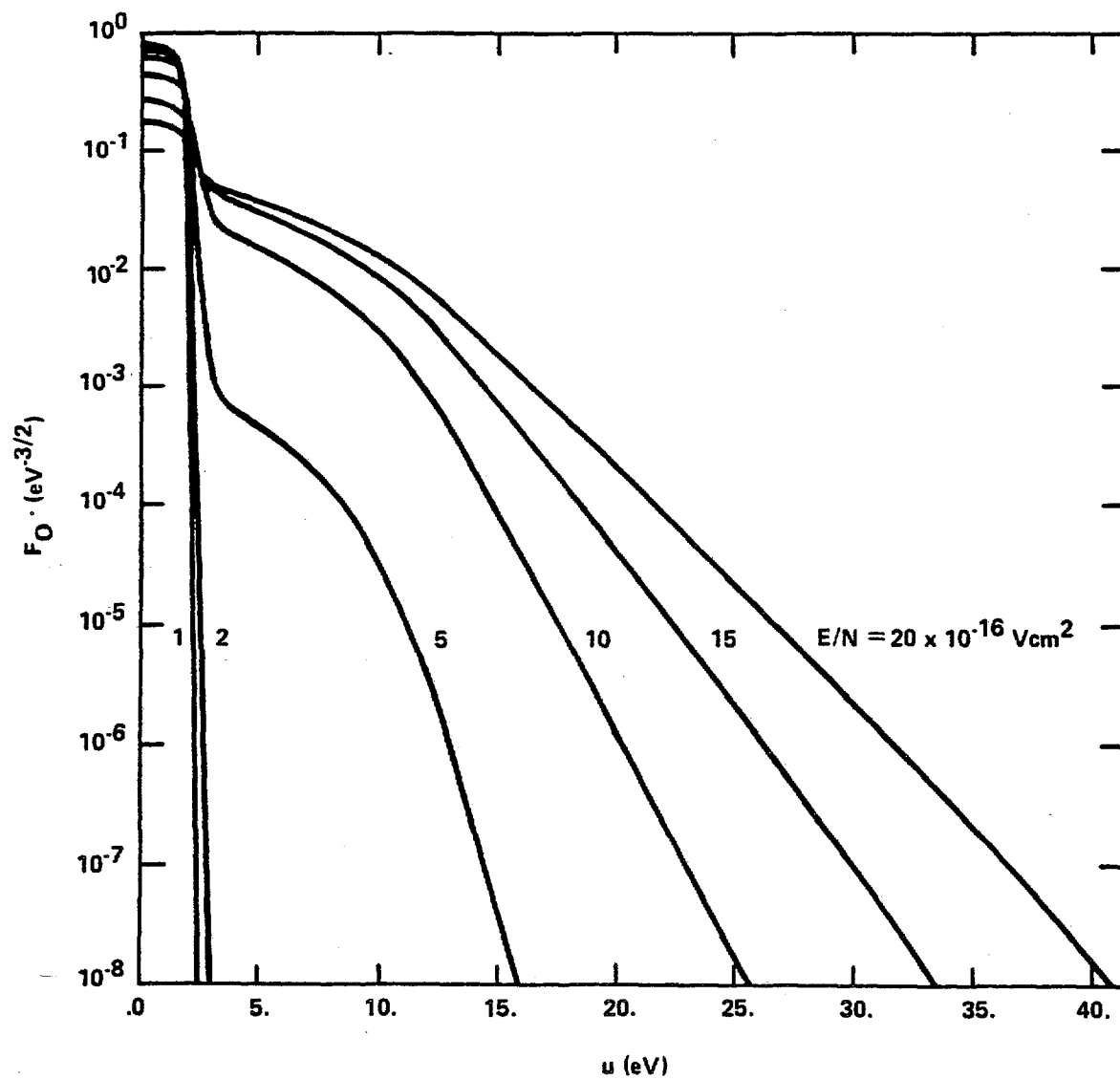


Figure 1

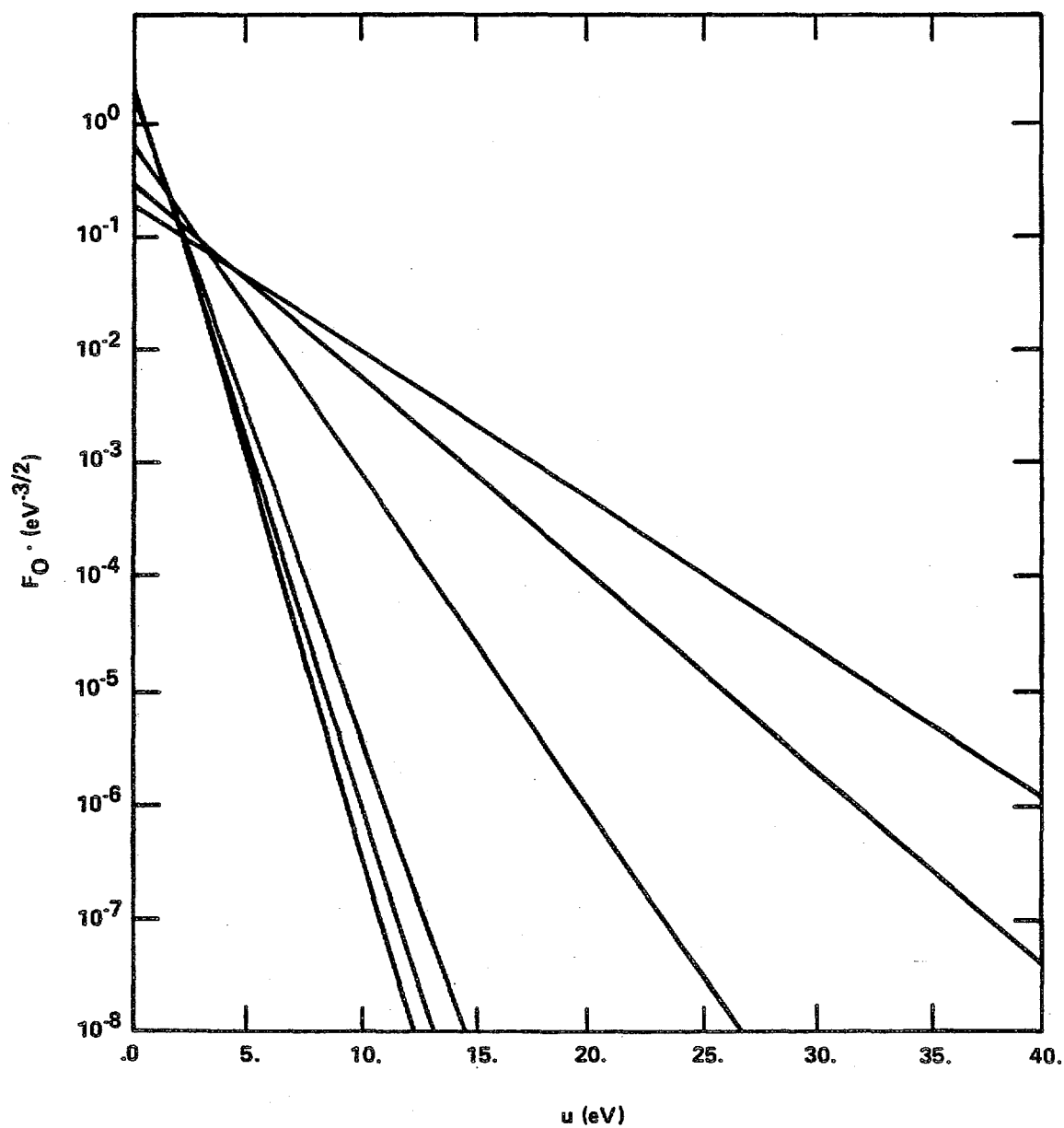


Figure 2
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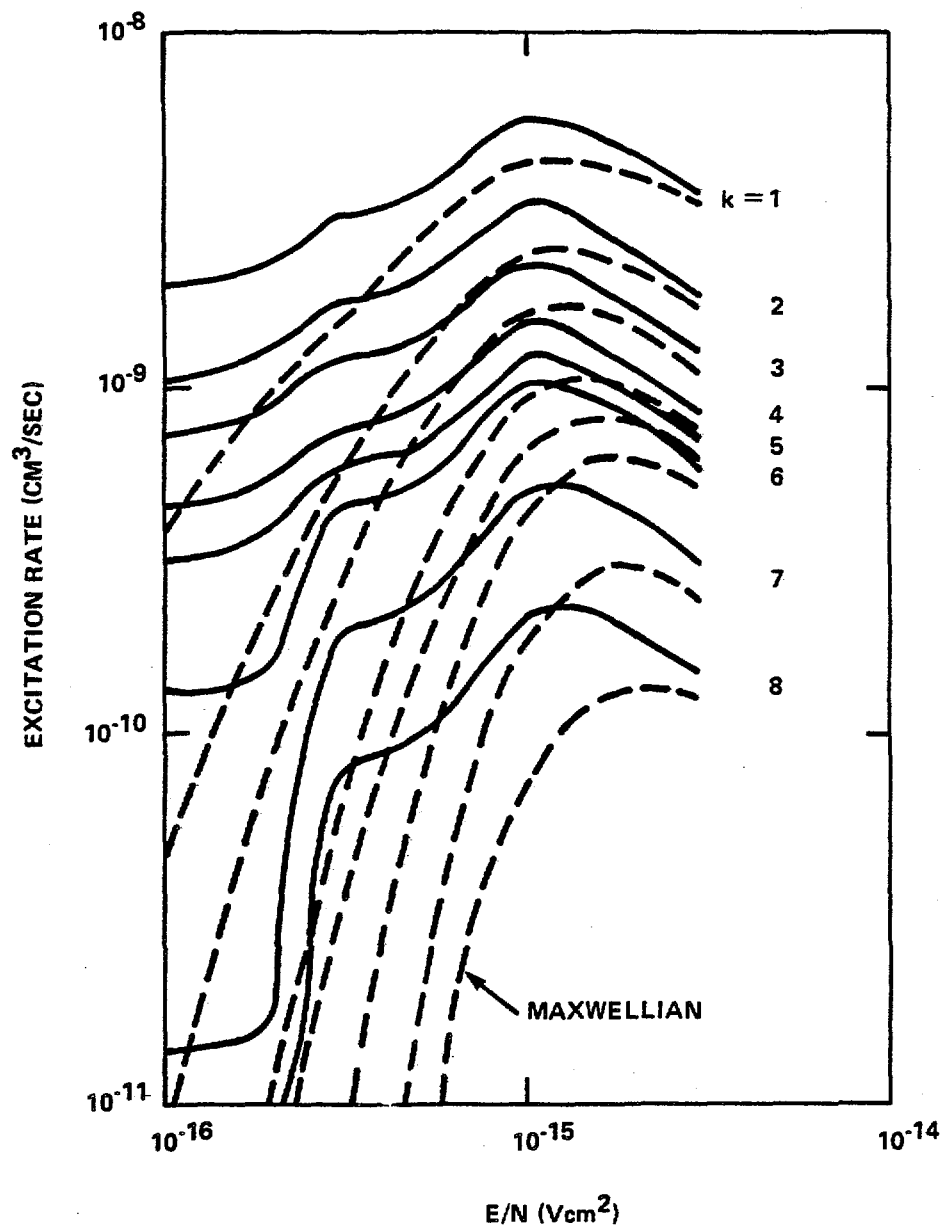


Figure 3

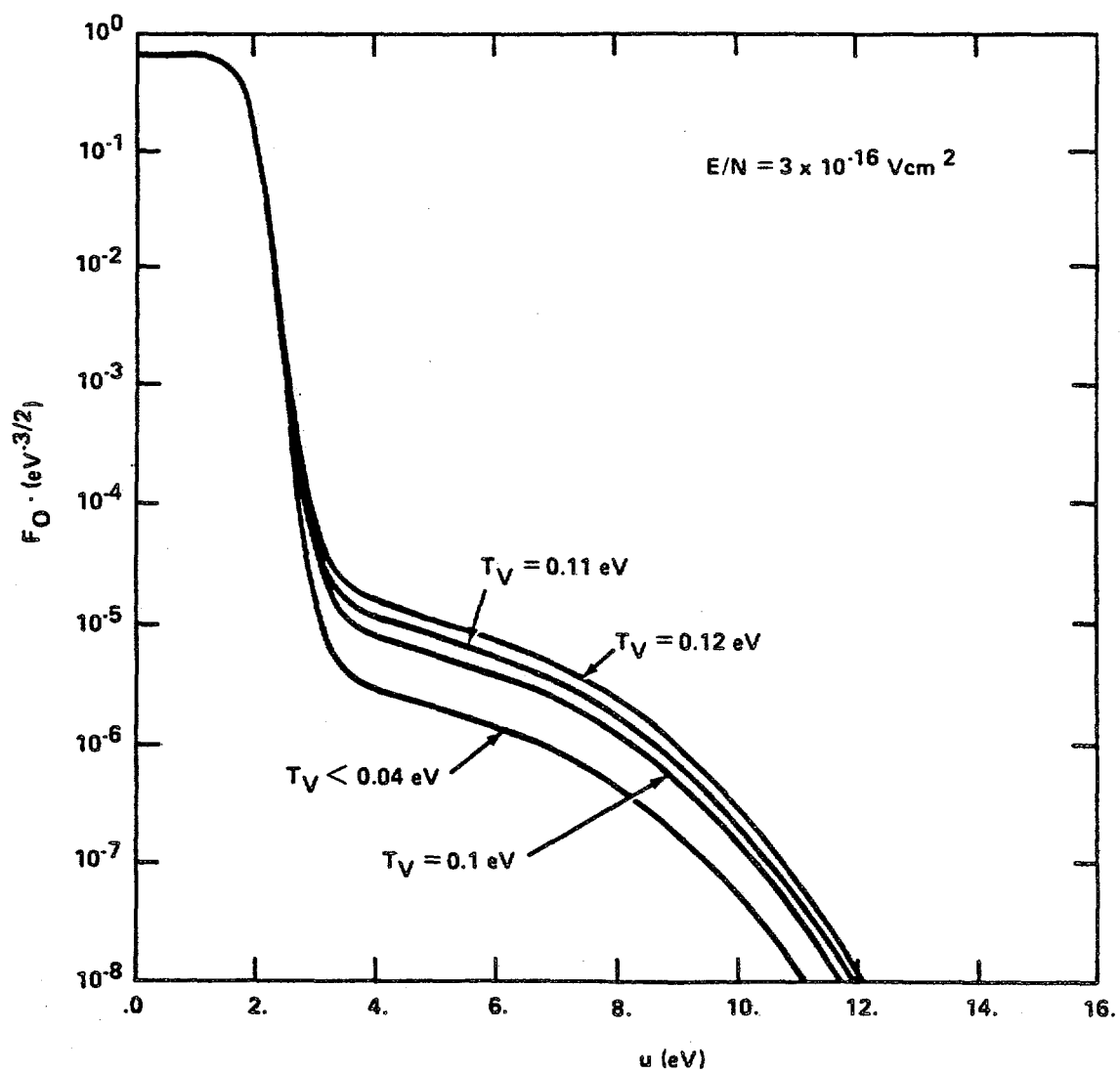


Figure 4

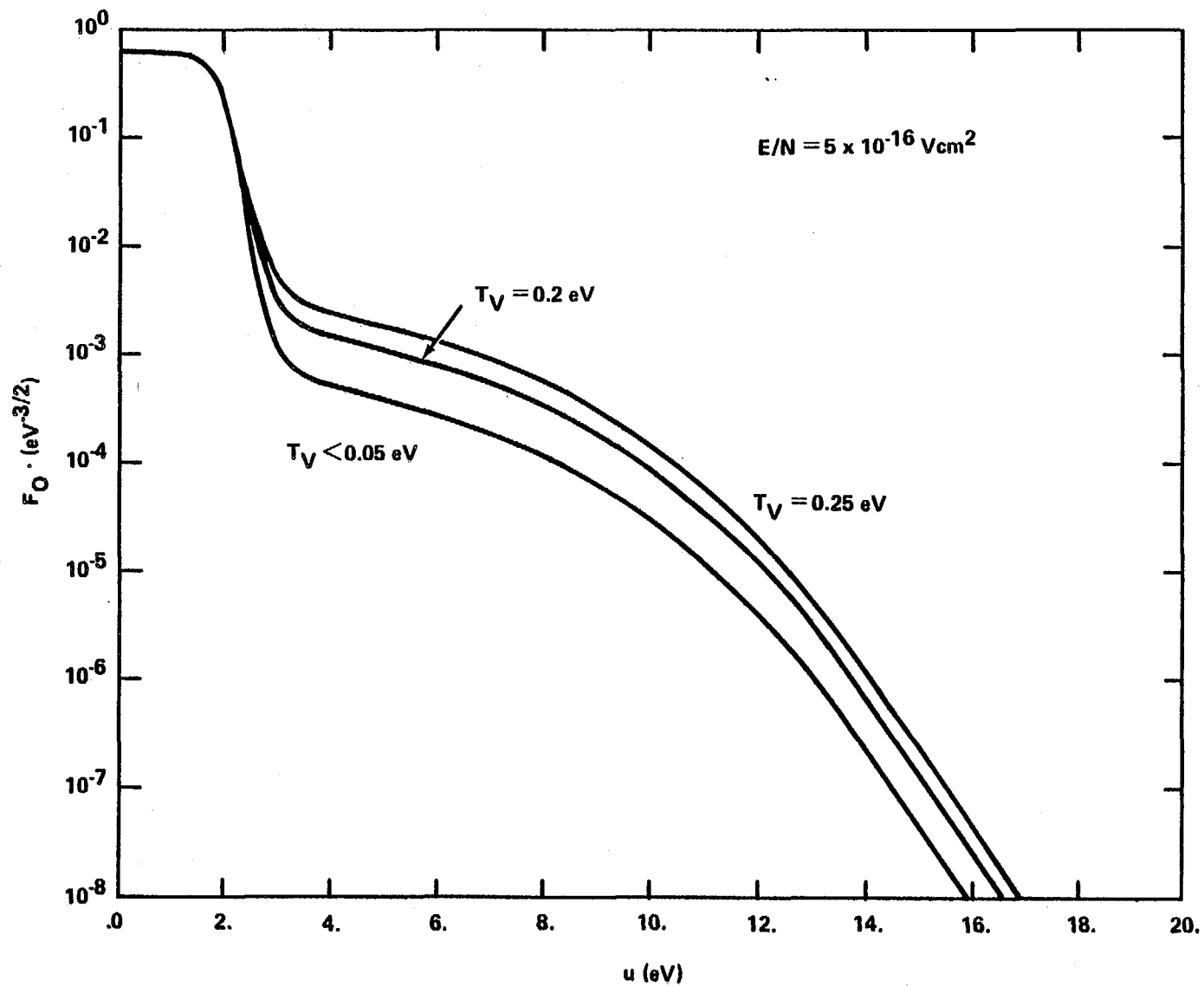


Figure 5

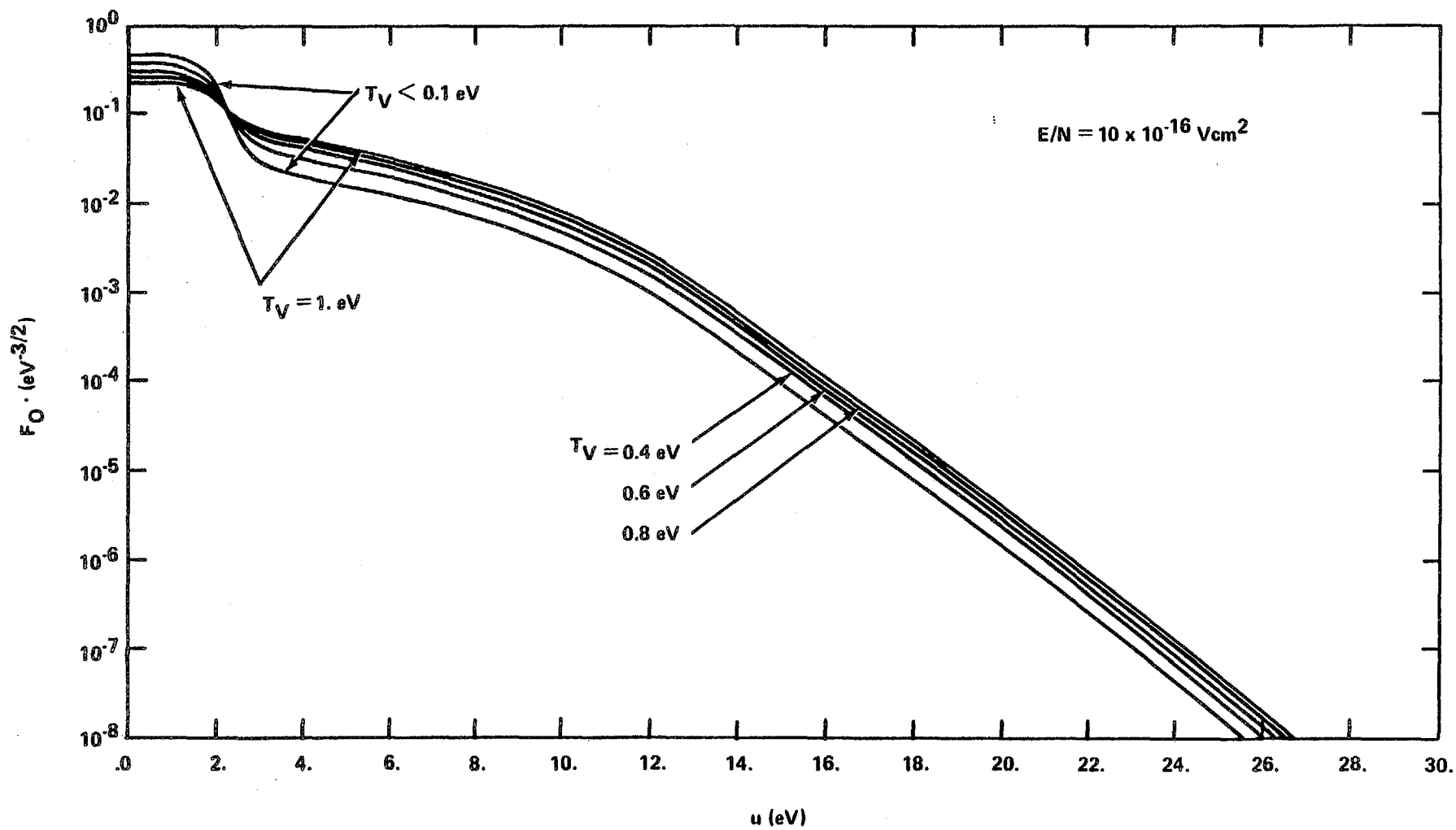


Figure 6

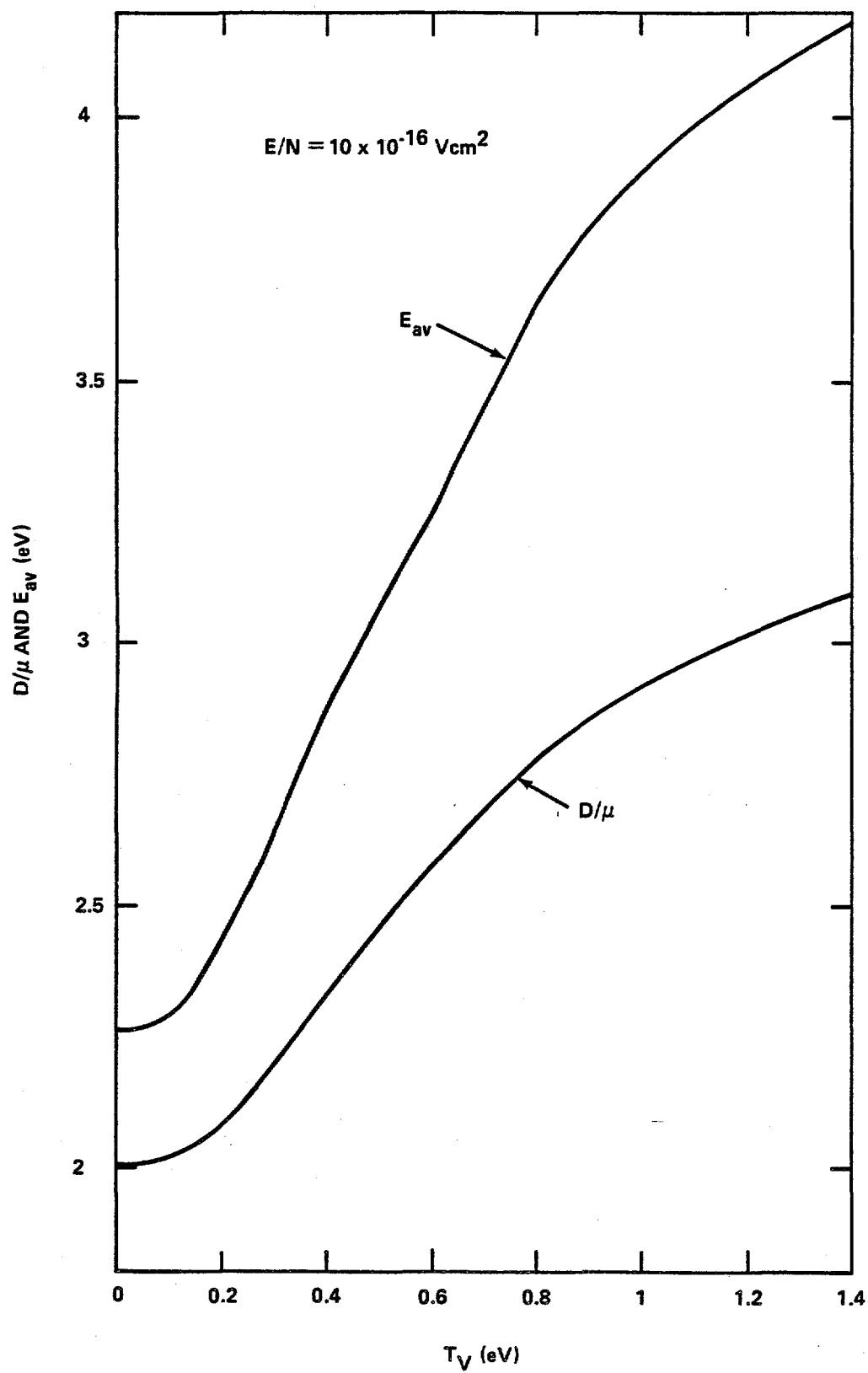


Figure 7
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